Full wwPDB EM Validation Report

Sep 3, 2022 – 08:45 am BST

PDB ID	:	7Z4H
EMDB ID	:	EMD-14497
Title	:	SpCas9 bound to 14-nucleotide complementary DNA substrate
Authors	:	Pacesa, M.; Jinek, M.
Deposited on	:	2022-03-03
Resolution	:	3.49 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

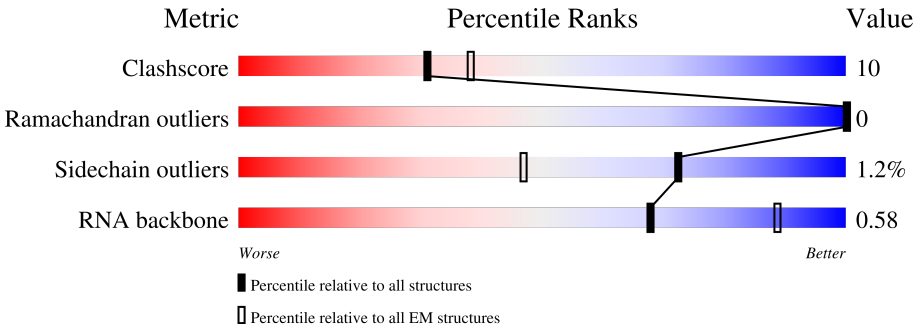
EMDB validation analysis	:	0.0.1.dev8
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.30

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.49 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	102	29% 48% 13% 10%
2	C	34	35% 56% 9%
3	D	34	18% 38% 44%
4	B	1368	11% 75% 22%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13900 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called sgRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A	92	1970	883	363	633	91	0	0

- Molecule 2 is a DNA chain called Target strand of 14-nucleotide complementary DNA substrate.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	C	31	625	301	107	187	30	0	0

- Molecule 3 is a DNA chain called Non-target strand of 14-nucleotide complementary DNA substrate.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	D	19	389	187	71	113	18	0	0

- Molecule 4 is a protein called CRISPR-associated endonuclease Cas9/Csn1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	B	1334	10916	6956	1894	2043	23	0	0

There are 2 discrepancies between the modelled and reference sequences:

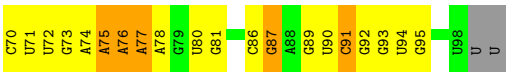
Chain	Residue	Modelled	Actual	Comment	Reference
B	10	ALA	ASP	engineered mutation	UNP Q99ZW2
B	840	ALA	HIS	engineered mutation	UNP Q99ZW2

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

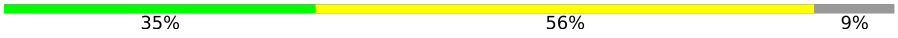
- Molecule 1: sgRNA

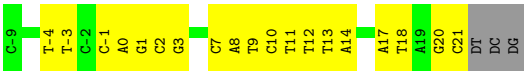
Chain A:



- Molecule 2: Target strand of 14-nucleotide complementary DNA substrate

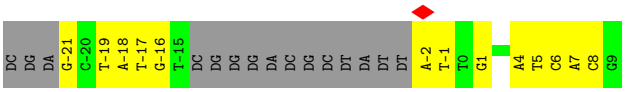
Chain C:





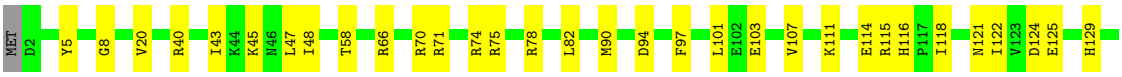
- Molecule 3: Non-target strand of 14-nucleotide complementary DNA substrate

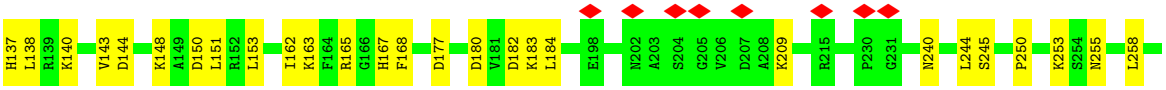
Chain D:

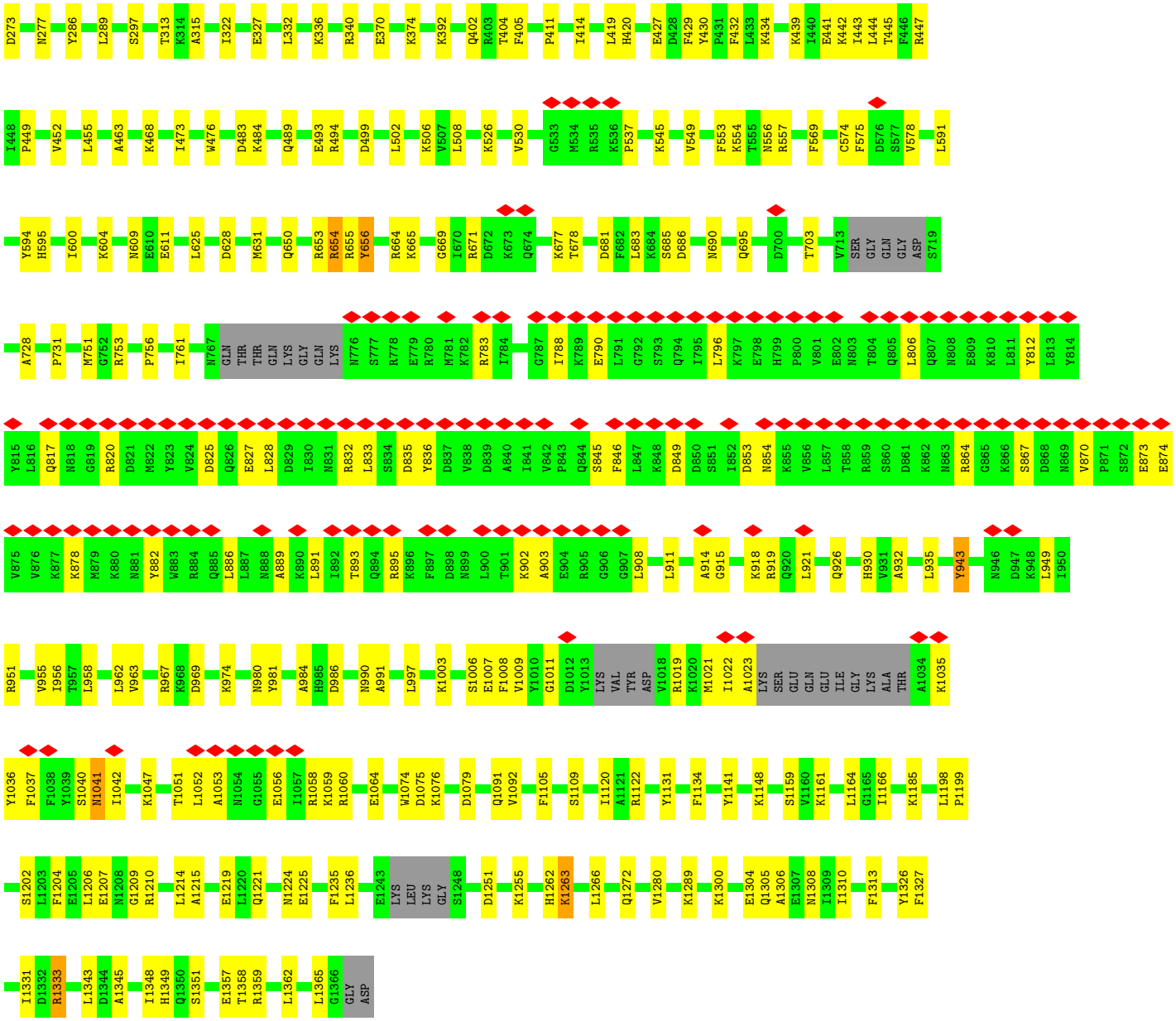


- Molecule 4: CRISPR-associated endonuclease Cas9/Csn1

Chain B:






D273 N277 Y286 L289 S297 T313 K314 A315 I322 E327 L332 K336 R340 E370 K374 K392 Q402 R403 T404 F405 P411 I414 L419 H420 E427 D428 F429 Y430 P431 F432 L433 K434 K439 I440 E441 K442 I443 L444 T445 F446 R447
I448 P449 V452 L455 A463 K468 I473 W476 D483 K484 Q489 E493 R494 D499 L502 K506 V507 L508 K526 V530 G533 M534 R535 K536 P537 K545 V549 F553 K554 T555 N556 R557 F569 C574 F575 D576 S577 V578 L591
Y594 H595 I600 K604 N609 E610 E611 L625 D628 M631 Q650 R653 R654 R655 Y656 R664 K665 G669 I670 R671 D672 K673 Q674 K677 T678 D681 F682 L683 K684 S685 D686 N690 Q695 D700 T703 V713 SER GLY GLN GLY ASP S719
A728 P731 M751 G752 R753 P756 I761 N767 GLN THR THR GLN LYS GLY GLN LYS N776 S777 R778 E779 R780 M781 K782 R783 I784 G787 I788 K789 E790 L791 G792 S793 Q794 I795 L796 K797 E798 H799 P800 V801 E802 N803 T804 Q805 L806 Q807 N808 E809 K810 L811 Y812 L813 Y814
Y815 L816 Q817 N818 G819 R820 D821 M822 Y823 V824 D825 Q826 E827 L828 D829 I830 N831 R832 L833 S834 D835 Y836 D837 V838 D839 A840 I841 V842 P843 Q844 S845 F846 L847 K848 D849 D850 S851 I852 D853 N854 K855 V856 L857 T858 R859 S860 D861 K862 N863 R864 G865 K866 S867 D868 N869 V870 P871 S872 E873 E874
V875 V876 K877 K878 M879 K880 N881 Y882 W883 R884 Q885 L886 L887 N888 A889 K890 L891 I892 T893 Q894 R895 K896 F897 D898 N899 L900 T901 K902 A903 E904 R905 G906 G907 L908 L911 A914 G915 K918 R919 Q920 L921 Q926 H930 V931 A932 L935 Y943 N946 D947 K948 L949 I950
R951 V955 I956 T957 L958 L962 V963 R967 K968 D969 K974 N980 Y981 A984 H985 D986 N990 A991 L997 K1003 S1006 E1007 F1008 V1009 Y1010 G1011 D1012 Y1013 LYS VAL TYR ASP V1018 R1019 K1020 M1021 I1022 A1023 LYS SER GLU GLN GLU ILE GLY LYS ALA THR A1034 K1035
Y1036 F1037 F1038 Y1039 S1040 N1041 I1042 K1047 T1051 L1052 A1053 N1054 G1055 E1056 I1057 R1058 K1059 R1060 E1064 W1074 D1075 K1076 D1079 Q1091 V1092 F1105 S1109 I1120 A1121 R1122 Y1131 F1134 Y1141 K1148 S1159 V1160 K1161 L1164 G1165 I1166 K1185 L1198 P1199
S1202 L1203 F1204 E1205 L1206 E1207 N1208 G1209 R1210 L1214 A1215 E1219 L1220 Q1221 N1224 E1225 F1235 L1236 E1243 LYS LEU LYS GLY S1248 D1251 K1255 H1262 K1263 L1266 Q1272 V1280 K1289 K1300 E1304 Q1305 A1306 E1307 N1308 I1309 I1310 F1313 Y1326 F1327
I1331 D1332 R1333 L1343 D1344 A1345 I1348 H1349 Q1350 S1351 E1357 T1358 R1359 L1362 L1365 G1366 GLY ASP

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	75738	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	67.44	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.176	Depositor
Minimum map value	-0.052	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.034	Depositor
Map size (Å)	249.59999, 249.59999, 249.59999	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.65, 0.65, 0.65	Depositor

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.30	0/2208	0.77	0/3441
2	C	0.52	0/698	0.95	0/1074
3	D	0.58	0/435	0.94	0/668
4	B	0.26	0/11107	0.45	0/14923
All	All	0.30	0/14448	0.58	0/20106

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1970	0	991	56	0
2	C	625	0	353	21	0
3	D	389	0	218	13	0
4	B	10916	0	11085	194	0
All	All	13900	0	12647	257	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (257) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:-21:DG:H5”	4:B:1006:SER:HB2	1.55	0.88
3:D:-2:DA:H1’	3:D:-1:DT:H5’	1.66	0.78
4:B:240:ASN:ND2	4:B:255:ASN:OD1	2.19	0.75
1:A:44:U:O2’	4:B:402:GLN:OE1	2.04	0.74
4:B:137:HIS:HA	4:B:322:ILE:HD11	1.73	0.71
4:B:180:ASP:HB2	4:B:184:LEU:HG	1.72	0.71
4:B:20:VAL:HB	4:B:47:LEU:HB3	1.73	0.71
1:A:94:U:H2’	1:A:95:G:H8	1.57	0.69
4:B:8:GLY:HA3	4:B:991:ALA:HB2	1.74	0.68
4:B:951:ARG:HH12	4:B:1011:GLY:HA3	1.59	0.68
4:B:82:LEU:HD22	4:B:162:ILE:HD12	1.75	0.68
1:A:61:C:OP1	4:B:70:ARG:NH2	2.24	0.67
4:B:1206:LEU:HD23	4:B:1345:ALA:HB2	1.76	0.67
4:B:569:PHE:HB3	4:B:575:PHE:HB2	1.75	0.67
4:B:864:ARG:HH11	4:B:867:SER:HA	1.59	0.66
2:C:-1:DC:H2”	2:C:0:DA:C8	2.32	0.65
4:B:846:PHE:HA	4:B:1040:SER:HB3	1.78	0.65
4:B:671:ARG:HG2	4:B:678:THR:HG22	1.78	0.65
4:B:849:ASP:HB3	4:B:854:ASN:HD22	1.62	0.65
4:B:140:LYS:NZ	4:B:144:ASP:OD2	2.30	0.63
4:B:820:ARG:NH2	4:B:825:ASP:OD1	2.31	0.63
4:B:1164:LEU:HD21	4:B:1185:LYS:HD3	1.81	0.63
1:A:75:A:H2’	1:A:76:A:C8	2.35	0.62
4:B:1300:LYS:O	4:B:1305:GLN:NE2	2.32	0.62
4:B:1051:THR:HG22	4:B:1053:ALA:H	1.64	0.62
2:C:2:DC:H2’	2:C:3:DG:H8	1.64	0.62
4:B:820:ARG:HG2	4:B:827:GLU:HG2	1.82	0.62
4:B:244:LEU:HB2	4:B:250:PRO:HG3	1.82	0.62
1:A:91:C:H5”	4:B:1091:GLN:HG3	1.81	0.61
4:B:508:LEU:HD21	4:B:664:ARG:HB2	1.82	0.61
4:B:1064:GLU:HB2	4:B:1074:TRP:HB3	1.83	0.61
1:A:46:A:H2’	1:A:47:A:H8	1.66	0.61
4:B:1023:ALA:HA	4:B:1035:LYS:HD3	1.83	0.61
4:B:783:ARG:NH2	4:B:891:LEU:O	2.34	0.61
4:B:182:ASP:OD1	4:B:209:LYS:NZ	2.34	0.60
4:B:427:GLU:HB2	4:B:434:LYS:HB2	1.81	0.60
4:B:1215:ALA:HB2	4:B:1221:GLN:HG3	1.83	0.60
4:B:820:ARG:HA	4:B:827:GLU:HA	1.84	0.60
4:B:914:ALA:HB2	4:B:1022:ILE:HD11	1.83	0.59
4:B:419:LEU:HD13	4:B:444:LEU:HD12	1.84	0.59
4:B:530:VAL:HG22	4:B:537:PRO:HB3	1.84	0.59
1:A:37:U:H2’	1:A:38:A:C8	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:545:LYS:NZ	4:B:683:LEU:O	2.36	0.58
3:D:6:DC:H2"	3:D:7:DA:C8	2.38	0.58
4:B:75:ARG:HA	4:B:78:ARG:HE	1.69	0.58
4:B:273:ASP:O	4:B:277:ASN:ND2	2.37	0.58
4:B:853:ASP:OD2	4:B:895:ARG:NH1	2.35	0.58
4:B:817:GLN:O	4:B:882:TYR:OH	2.23	0.57
3:D:-19:DT:H2'	3:D:-18:DA:C8	2.40	0.57
1:A:45:U:H2'	1:A:46:A:H8	1.70	0.57
1:A:37:U:H2'	1:A:38:A:H8	1.69	0.57
1:A:94:U:H2'	1:A:95:G:C8	2.39	0.57
4:B:853:ASP:OD1	4:B:893:THR:OG1	2.21	0.57
4:B:180:ASP:HB3	4:B:183:LYS:HB2	1.88	0.56
4:B:370:GLU:OE2	4:B:374:LYS:NZ	2.39	0.56
1:A:17:A:OP2	4:B:74:ARG:NH1	2.34	0.56
4:B:956:ILE:HG12	4:B:1009:VAL:HG22	1.87	0.56
4:B:1075:ASP:N	4:B:1079:ASP:OD2	2.30	0.56
1:A:46:A:H2'	1:A:47:A:C8	2.41	0.55
4:B:761:ILE:CD1	4:B:955:VAL:HG13	2.37	0.55
3:D:4:DA:H2'	3:D:5:DT:H71	1.89	0.55
4:B:788:ILE:HG12	4:B:796:LEU:HG	1.89	0.55
1:A:56:U:O2'	1:A:58:G:N2	2.40	0.55
3:D:-18:DA:H3'	3:D:-17:DT:H71	1.88	0.55
4:B:981:TYR:CE1	4:B:1092:VAL:HB	2.42	0.55
4:B:980:ASN:ND2	4:B:1225:GLU:OE2	2.40	0.55
3:D:-19:DT:H2'	3:D:-18:DA:H8	1.71	0.55
3:D:1:DG:N7	4:B:1333:ARG:NH2	2.55	0.55
2:C:-4:DT:H1'	2:C:-3:DT:H5'	1.88	0.54
4:B:286:TYR:O	4:B:289:LEU:HB3	2.08	0.54
2:C:7:DC:H2'	2:C:8:DA:H8	1.73	0.54
4:B:209:LYS:HZ2	4:B:209:LYS:HB2	1.73	0.53
4:B:468:LYS:HE3	4:B:483:ASP:HA	1.90	0.53
4:B:499:ASP:OD2	4:B:502:LEU:N	2.41	0.53
4:B:1349:HIS:HB2	4:B:1358:THR:HB	1.89	0.53
4:B:556:ASN:O	4:B:595:HIS:NE2	2.41	0.53
4:B:686:ASP:HB3	4:B:690:ASN:HA	1.91	0.53
1:A:54:G:H2'	1:A:55:C:C6	2.44	0.52
4:B:420:HIS:ND1	4:B:441:GLU:OE2	2.41	0.52
4:B:967:ARG:NH1	4:B:986:ASP:OD1	2.43	0.52
4:B:1021:MET:HG3	4:B:1036:TYR:HB2	1.91	0.52
4:B:1161:LYS:HE3	4:B:1343:LEU:HB3	1.91	0.52
2:C:20:DG:H4'	4:B:695:GLN:HE21	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:75:ARG:HB2	4:B:78:ARG:HH21	1.75	0.52
2:C:8:DA:H2'	2:C:9:DT:H6	1.75	0.51
2:C:8:DA:H2'	2:C:9:DT:C6	2.46	0.51
4:B:833:LEU:HD23	4:B:836:TYR:HD2	1.76	0.51
2:C:11:DT:H2"	4:B:728:ALA:HB1	1.92	0.51
1:A:40:C:OP1	4:B:340:ARG:NH1	2.37	0.51
4:B:926:GLN:O	4:B:930:HIS:ND1	2.30	0.51
1:A:18:C:H41	4:B:71:ARG:NH2	2.09	0.51
2:C:1:DG:OP2	4:B:1109:SER:N	2.44	0.51
4:B:1209:GLY:O	4:B:1224:ASN:ND2	2.43	0.51
4:B:493:GLU:HB3	4:B:506:LYS:NZ	2.26	0.50
4:B:958:LEU:HD11	4:B:962:LEU:HD23	1.93	0.50
1:A:47:A:H4'	4:B:101:LEU:HD22	1.93	0.50
4:B:665:LYS:HA	4:B:669:GLY:HA3	1.92	0.50
4:B:168:PHE:CD1	4:B:447:ARG:HD3	2.46	0.50
4:B:121:ASN:ND2	4:B:124:ASP:OD2	2.39	0.50
4:B:463:ALA:O	4:B:494:ARG:NH1	2.44	0.50
4:B:530:VAL:O	4:B:578:VAL:HA	2.11	0.50
1:A:21:G:H1'	2:C:1:DG:N2	2.26	0.50
1:A:43:G:N7	4:B:336:LYS:NZ	2.54	0.50
4:B:443:ILE:HD11	4:B:476:TRP:HZ2	1.76	0.50
4:B:1308:ASN:OD1	4:B:1327:PHE:N	2.43	0.50
1:A:47:A:O2'	4:B:101:LEU:O	2.28	0.49
4:B:870:VAL:HG23	4:B:908:LEU:HB2	1.94	0.49
4:B:411:PRO:HG2	4:B:414:ILE:HG12	1.93	0.49
4:B:554:LYS:HB3	4:B:604:LYS:HZ1	1.78	0.49
4:B:677:LYS:HB3	4:B:681:ASP:HB2	1.94	0.49
2:C:9:DT:H2'	2:C:10:DC:H6	1.77	0.49
3:D:7:DA:H2"	3:D:8:DC:H2'	1.94	0.49
1:A:22:U:H2'	1:A:23:U:H6	1.78	0.49
4:B:967:ARG:NH2	4:B:974:LYS:HB3	2.28	0.49
4:B:969:ASP:HB3	4:B:1047:LYS:NZ	2.27	0.49
1:A:92:G:OP1	4:B:40:ARG:NH1	2.45	0.49
1:A:53:G:H2'	1:A:54:G:H8	1.77	0.49
1:A:90:U:O2	4:B:981:TYR:OH	2.31	0.49
2:C:7:DC:H2'	2:C:8:DA:C8	2.48	0.49
4:B:1120:ILE:N	4:B:1134:PHE:O	2.38	0.49
2:C:17:DA:H3'	2:C:18:DT:H71	1.95	0.48
4:B:48:ILE:HG12	4:B:984:ALA:HB1	1.96	0.48
4:B:327:GLU:OE1	4:B:392:LYS:NZ	2.44	0.48
4:B:870:VAL:HG11	4:B:902:LYS:HB3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:874:GLU:HG2	4:B:878:LYS:HE3	1.95	0.48
4:B:943:TYR:HA	4:B:949:LEU:HA	1.94	0.48
4:B:1310:ILE:HA	4:B:1313:PHE:HD2	1.78	0.48
4:B:439:LYS:HG2	4:B:476:TRP:CD1	2.49	0.48
4:B:1198:LEU:HD13	4:B:1204:PHE:HZ	1.79	0.48
1:A:45:U:H2'	1:A:46:A:C8	2.48	0.47
2:C:2:DC:H2'	2:C:3:DG:C8	2.46	0.47
2:C:9:DT:H2'	2:C:10:DC:C6	2.49	0.47
4:B:549:VAL:HA	4:B:553:PHE:HD2	1.79	0.47
1:A:11:G:H2'	1:A:12:A:H8	1.79	0.47
1:A:43:G:H3'	1:A:44:U:C6	2.50	0.47
1:A:61:C:P	4:B:70:ARG:HH21	2.36	0.47
4:B:1308:ASN:HB3	4:B:1326:TYR:CD1	2.50	0.47
1:A:73:G:O2'	1:A:75:A:N6	2.40	0.47
4:B:442:LYS:HA	4:B:445:THR:HG22	1.96	0.47
4:B:790:GLU:HG2	4:B:889:ALA:HA	1.96	0.47
4:B:915:GLY:O	4:B:919:ARG:HG2	2.14	0.47
4:B:107:VAL:HG13	4:B:1131:TYR:CE1	2.49	0.47
4:B:138:LEU:HD11	4:B:153:LEU:HB3	1.97	0.47
2:C:12:DT:H2'	2:C:13:DT:C6	2.51	0.46
1:A:86:C:H2'	1:A:87:G:O4'	2.16	0.46
4:B:125:GLU:OE2	4:B:129:HIS:NE2	2.45	0.46
4:B:1210:ARG:HA	4:B:1280:VAL:HG13	1.97	0.46
2:C:11:DT:H3'	2:C:12:DT:H71	1.96	0.46
4:B:591:LEU:HB3	4:B:594:TYR:HB3	1.98	0.46
1:A:91:C:H2'	1:A:92:G:H8	1.79	0.46
1:A:24:U:H2'	1:A:25:U:C6	2.50	0.46
1:A:34:A:H3'	1:A:35:A:H8	1.80	0.46
2:C:10:DC:H3'	2:C:11:DT:H71	1.98	0.46
2:C:13:DT:C2	2:C:14:DA:C8	3.04	0.46
4:B:103:GLU:O	4:B:111:LYS:NZ	2.48	0.46
4:B:137:HIS:CE1	4:B:322:ILE:HG12	2.51	0.46
4:B:58:THR:HA	4:B:731:PRO:HG2	1.98	0.46
4:B:921:LEU:HD13	4:B:921:LEU:HA	1.76	0.46
4:B:5:TYR:CE2	4:B:756:PRO:HB3	2.51	0.45
4:B:628:ASP:OD2	4:B:631:MET:HG2	2.16	0.45
1:A:22:U:H2'	1:A:23:U:C6	2.52	0.45
1:A:48:A:OP2	4:B:163:LYS:NZ	2.43	0.45
4:B:114:GLU:OE1	4:B:116:HIS:N	2.29	0.45
4:B:609:ASN:HD21	4:B:611:GLU:HB2	1.81	0.45
4:B:761:ILE:HD13	4:B:955:VAL:HG13	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:-17:DT:H2'	3:D:-16:DG:C8	2.52	0.45
4:B:1304:GLU:O	4:B:1308:ASN:ND2	2.33	0.45
4:B:148:LYS:HB2	4:B:429:PHE:CD1	2.52	0.45
4:B:956:ILE:HG23	4:B:1008:PHE:HD2	1.81	0.45
1:A:27:G:OP2	4:B:115:ARG:NH1	2.49	0.45
4:B:66:ARG:HG2	4:B:70:ARG:NH1	2.32	0.45
4:B:90:MET:O	4:B:94:ASP:N	2.46	0.45
4:B:1148:LYS:HG3	4:B:1159:SER:HA	1.99	0.45
4:B:1362:LEU:HA	4:B:1365:LEU:HD13	1.98	0.45
1:A:10:A:H2'	1:A:11:G:C8	2.51	0.45
4:B:43:ILE:HD13	4:B:45:LYS:HE2	1.98	0.45
4:B:332:LEU:HD11	4:B:336:LYS:HE3	1.99	0.44
4:B:677:LYS:NZ	4:B:685:SER:O	2.49	0.44
4:B:1357:GLU:OE1	4:B:1359:ARG:NH1	2.49	0.44
4:B:253:LYS:HG3	4:B:258:LEU:O	2.17	0.44
4:B:557:ARG:HA	4:B:595:HIS:CD2	2.52	0.44
4:B:526:LYS:HA	4:B:526:LYS:HD3	1.77	0.44
4:B:783:ARG:NH1	4:B:812:TYR:OH	2.49	0.44
4:B:932:ALA:HA	4:B:955:VAL:HG11	2.00	0.44
4:B:455:LEU:HB3	4:B:473:ILE:HD12	2.00	0.44
1:A:20:C:C2	1:A:21:G:C8	3.05	0.44
1:A:77:A:H2'	1:A:78:A:H8	1.82	0.44
4:B:918:LYS:NZ	4:B:1007:GLU:OE2	2.49	0.44
4:B:870:VAL:HG21	4:B:902:LYS:HD3	2.00	0.43
3:D:1:DG:OP2	4:B:1221:GLN:NE2	2.48	0.43
4:B:828:LEU:HB3	4:B:836:TYR:CE2	2.53	0.43
4:B:963:VAL:HG21	4:B:990:ASN:OD1	2.19	0.43
1:A:53:G:H2'	1:A:54:G:C8	2.54	0.43
3:D:1:DG:H2'	4:B:1219:GLU:OE1	2.19	0.43
4:B:832:ARG:NH1	4:B:835:ASP:OD2	2.52	0.43
1:A:80:U:OP2	4:B:753:ARG:NH2	2.52	0.43
1:A:93:G:H2'	1:A:94:U:C6	2.54	0.43
4:B:1236:LEU:HB3	4:B:1310:ILE:HD11	2.00	0.43
1:A:72:U:H2'	1:A:73:G:O4'	2.19	0.43
4:B:182:ASP:OD1	4:B:209:LYS:HB2	2.19	0.43
4:B:886:LEU:HD22	4:B:891:LEU:HD12	1.99	0.43
4:B:997:LEU:HD11	4:B:1042:ILE:HG13	2.00	0.43
4:B:1348:ILE:HG12	4:B:1359:ARG:HG2	2.00	0.43
1:A:68:A:C8	4:B:1351:SER:HA	2.54	0.43
1:A:29:G:C6	1:A:41:A:C6	3.07	0.43
4:B:449:PRO:HB2	4:B:452:VAL:HG23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:245:SER:HA	4:B:297:SER:HB2	2.01	0.43
4:B:1058:ARG:HG2	4:B:1059:LYS:H	1.83	0.43
4:B:177:ASP:N	4:B:177:ASP:OD1	2.52	0.42
2:C:12:DT:H2'	2:C:13:DT:H6	1.85	0.42
3:D:-2:DA:H2'	3:D:-1:DT:H72	2.01	0.42
4:B:1251:ASP:HB3	4:B:1255:LYS:NZ	2.34	0.42
1:A:77:A:H2'	1:A:78:A:C8	2.54	0.42
4:B:569:PHE:O	4:B:574:CYS:N	2.52	0.42
4:B:1263:LYS:O	4:B:1266:LEU:HB2	2.19	0.42
4:B:1207:GLU:OE2	4:B:1210:ARG:NH2	2.44	0.42
4:B:1235:PHE:CD1	4:B:1262:HIS:HB2	2.54	0.42
4:B:97:PHE:HE1	4:B:118:ILE:HA	1.85	0.42
4:B:143:VAL:HG11	4:B:315:ALA:HB2	2.01	0.42
4:B:963:VAL:O	4:B:967:ARG:HG3	2.19	0.42
4:B:1199:PRO:O	4:B:1202:SER:OG	2.28	0.42
4:B:144:ASP:OD1	4:B:313:THR:OG1	2.34	0.42
4:B:484:LYS:HB3	4:B:484:LYS:HE3	1.86	0.42
4:B:1333:ARG:H	4:B:1333:ARG:HG2	1.69	0.42
4:B:439:LYS:HG2	4:B:476:TRP:NE1	2.34	0.42
4:B:493:GLU:HB3	4:B:506:LYS:HZ3	1.85	0.42
4:B:1289:LYS:HE3	4:B:1331:ILE:HD12	2.01	0.42
1:A:38:A:H2'	1:A:39:G:C8	2.55	0.41
1:A:49:A:N3	4:B:1122:ARG:NH2	2.67	0.41
1:A:93:G:H2'	1:A:94:U:H6	1.85	0.41
4:B:935:LEU:HD23	4:B:935:LEU:HA	1.76	0.41
1:A:11:G:H2'	1:A:12:A:C8	2.55	0.41
2:C:20:DG:H3'	2:C:21:DC:C5	2.56	0.41
4:B:845:SER:O	4:B:1041:ASN:N	2.54	0.41
1:A:18:C:OP1	4:B:165:ARG:NE	2.45	0.41
1:A:22:U:C2	1:A:23:U:C5	3.09	0.41
1:A:33:G:N2	1:A:36:A:OP2	2.42	0.41
4:B:430:TYR:HB3	4:B:432:PHE:CE1	2.55	0.41
4:B:489:GLN:HG3	4:B:625:LEU:HD13	2.03	0.41
4:B:1022:ILE:HD12	4:B:1022:ILE:H	1.85	0.41
4:B:404:THR:HG22	4:B:405:PHE:H	1.85	0.41
4:B:600:ILE:HG23	4:B:650:GLN:HE21	1.85	0.41
4:B:873:GLU:HG2	4:B:903:ALA:HB1	2.03	0.41
4:B:911:LEU:HB2	4:B:1019:ARG:HH21	1.86	0.41
4:B:5:TYR:CZ	4:B:751:MET:HG3	2.56	0.41
4:B:150:ASP:OD1	4:B:151:LEU:N	2.54	0.41
4:B:654:ARG:HD3	4:B:656:TYR:CE2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:1052:LEU:HB2	4:B:1056:GLU:HB2	2.02	0.41
1:A:70:C:C2	1:A:71:U:C5	3.09	0.40
4:B:1060:ARG:HB2	4:B:1076:LYS:HZ1	1.86	0.40
4:B:107:VAL:HG22	4:B:1131:TYR:OH	2.22	0.40
4:B:806:LEU:HD23	4:B:806:LEU:HA	1.93	0.40
4:B:1204:PHE:HE1	4:B:1214:LEU:HB2	1.87	0.40
1:A:41:A:H2'	1:A:42:A:C8	2.56	0.40
4:B:1306:ALA:O	4:B:1310:ILE:HG12	2.21	0.40
1:A:52:A:C8	4:B:1105:PHE:HE2	2.39	0.40
4:B:1141:TYR:O	4:B:1166:ILE:HB	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	B	1322/1368 (97%)	1295 (98%)	27 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	B	1198/1225 (98%)	1184 (99%)	14 (1%)	71	87

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	B	122	ILE
4	B	167	HIS
4	B	653	ARG
4	B	654	ARG
4	B	655	ARG
4	B	656	TYR
4	B	703	THR
4	B	943	TYR
4	B	1003	LYS
4	B	1037	PHE
4	B	1041	ASN
4	B	1263	LYS
4	B	1272	GLN
4	B	1333	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
4	B	739	GLN
4	B	1241	HIS
4	B	1262	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	91/102 (89%)	20 (21%)	0

All (20) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	10	A
1	A	17	A
1	A	28	A
1	A	29	G
1	A	34	A
1	A	37	U
1	A	38	A
1	A	51	A
1	A	53	G

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Mol	Chain	Res	Type
1	A	57	A
1	A	59	U
1	A	68	A
1	A	74	A
1	A	75	A
1	A	76	A
1	A	77	A
1	A	81	G
1	A	87	G
1	A	89	G
1	A	91	C

There are no RNA pucker outliers to report.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

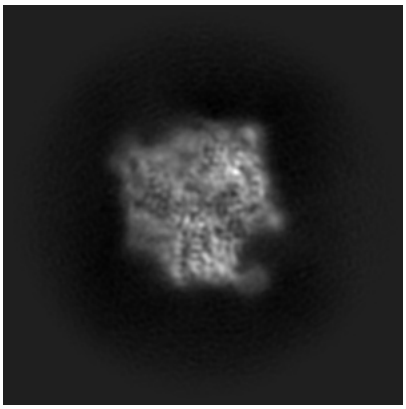
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-14497. These allow visual inspection of the internal detail of the map and identification of artifacts.

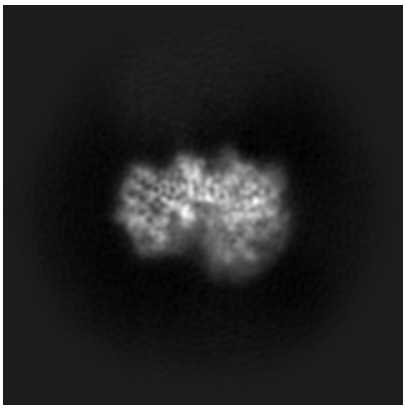
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

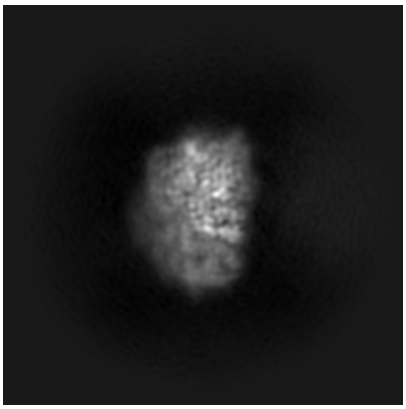
6.1.1 Primary map



X

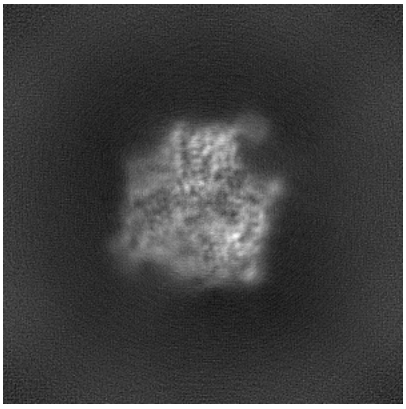


Y

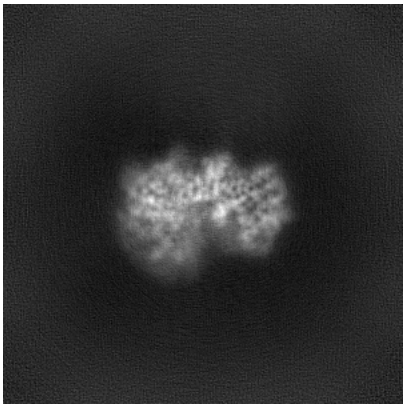


Z

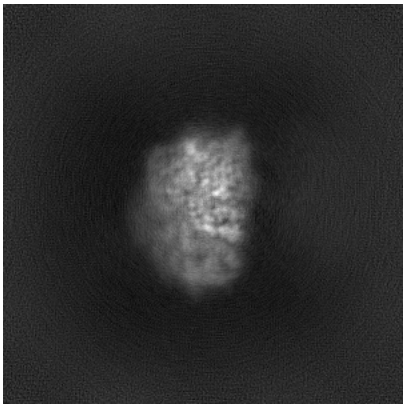
6.1.2 Raw map



X



Y

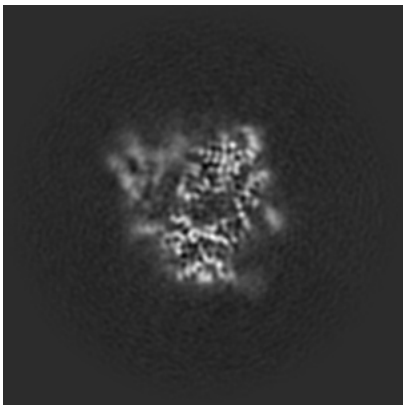


Z

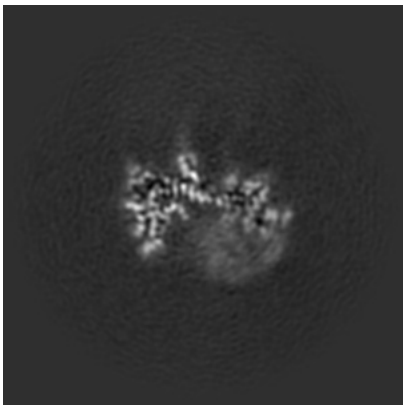
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

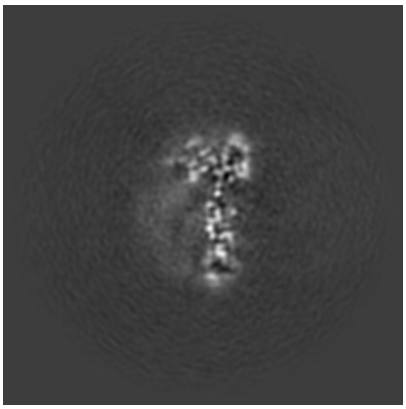
6.2.1 Primary map



X Index: 192

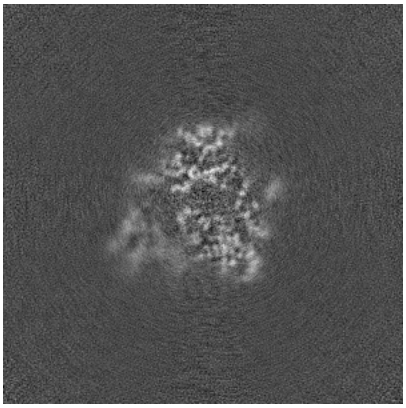


Y Index: 192

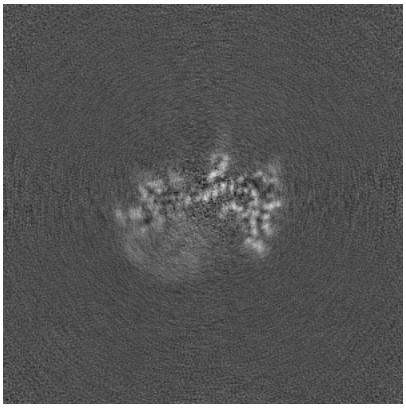


Z Index: 192

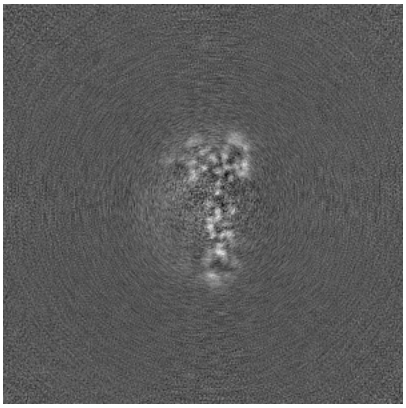
6.2.2 Raw map



X Index: 192



Y Index: 192

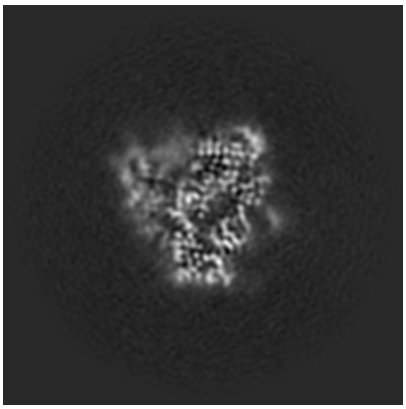


Z Index: 192

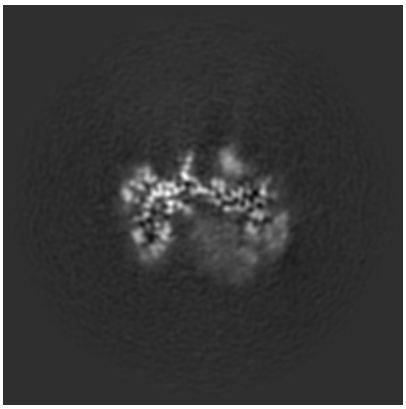
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

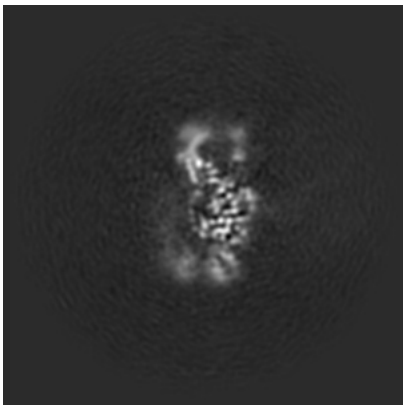
6.3.1 Primary map



X Index: 196

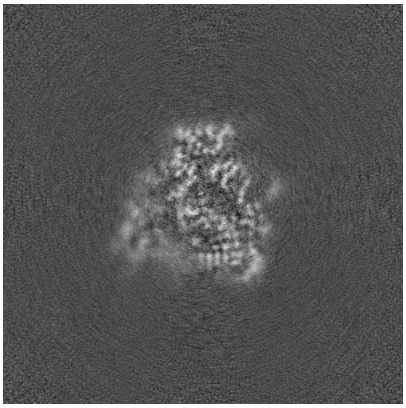


Y Index: 202

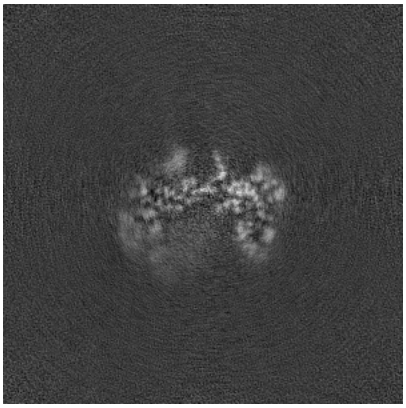


Z Index: 179

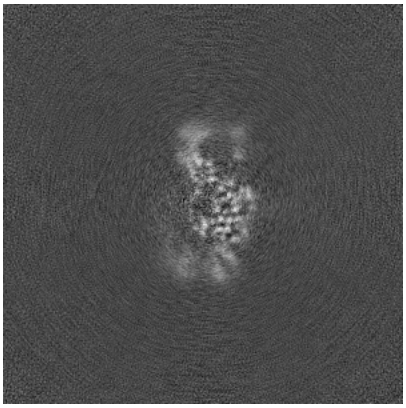
6.3.2 Raw map



X Index: 195



Y Index: 202

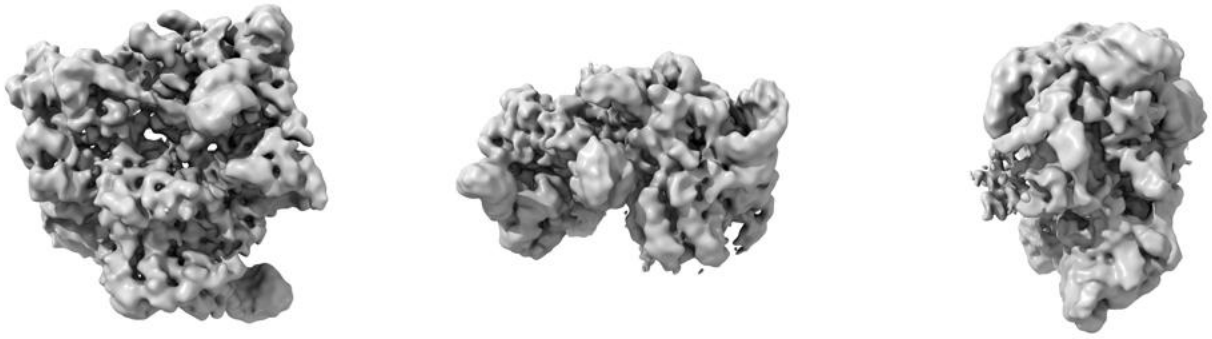


Z Index: 206

The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.034. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map

X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

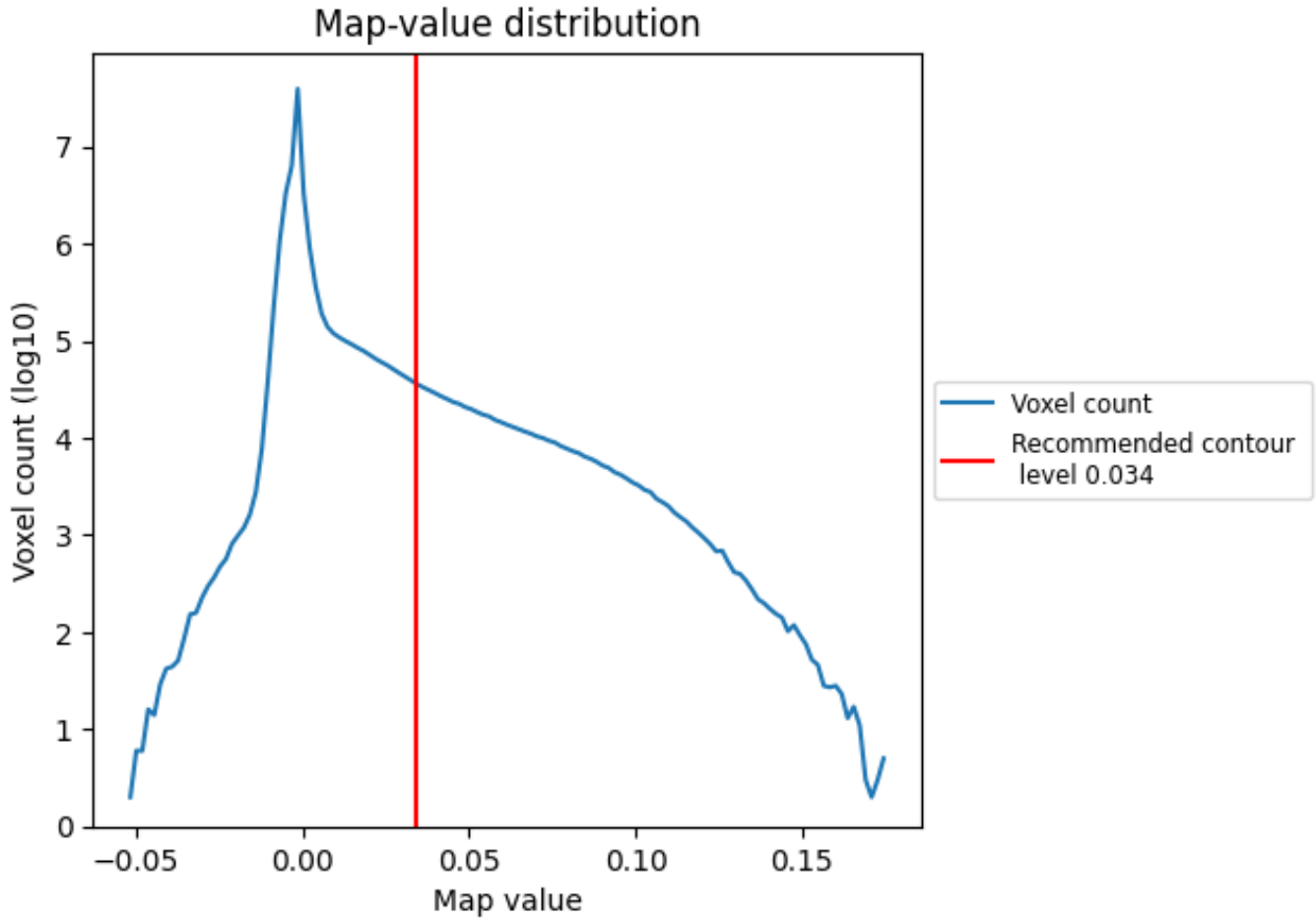
6.5 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

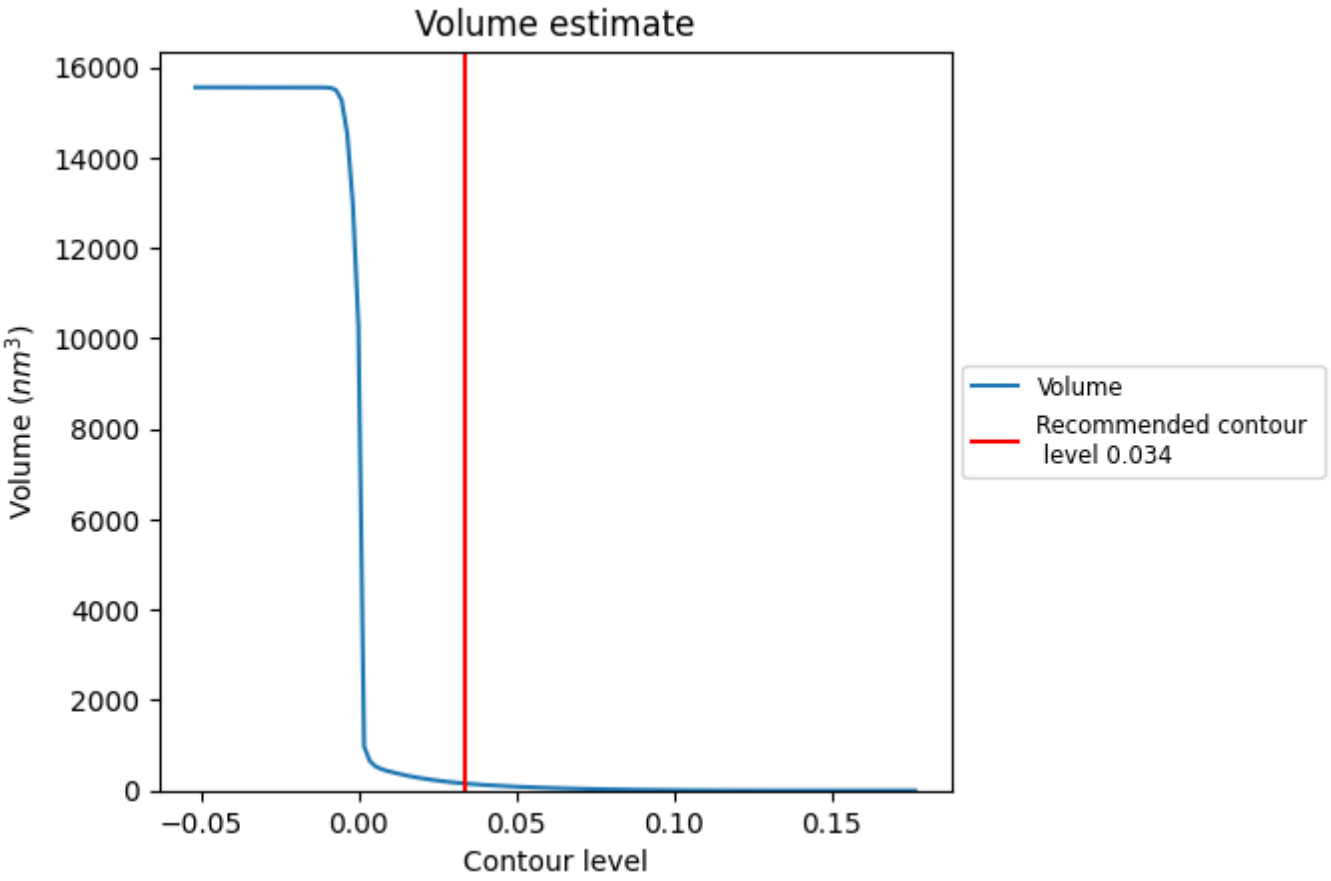
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

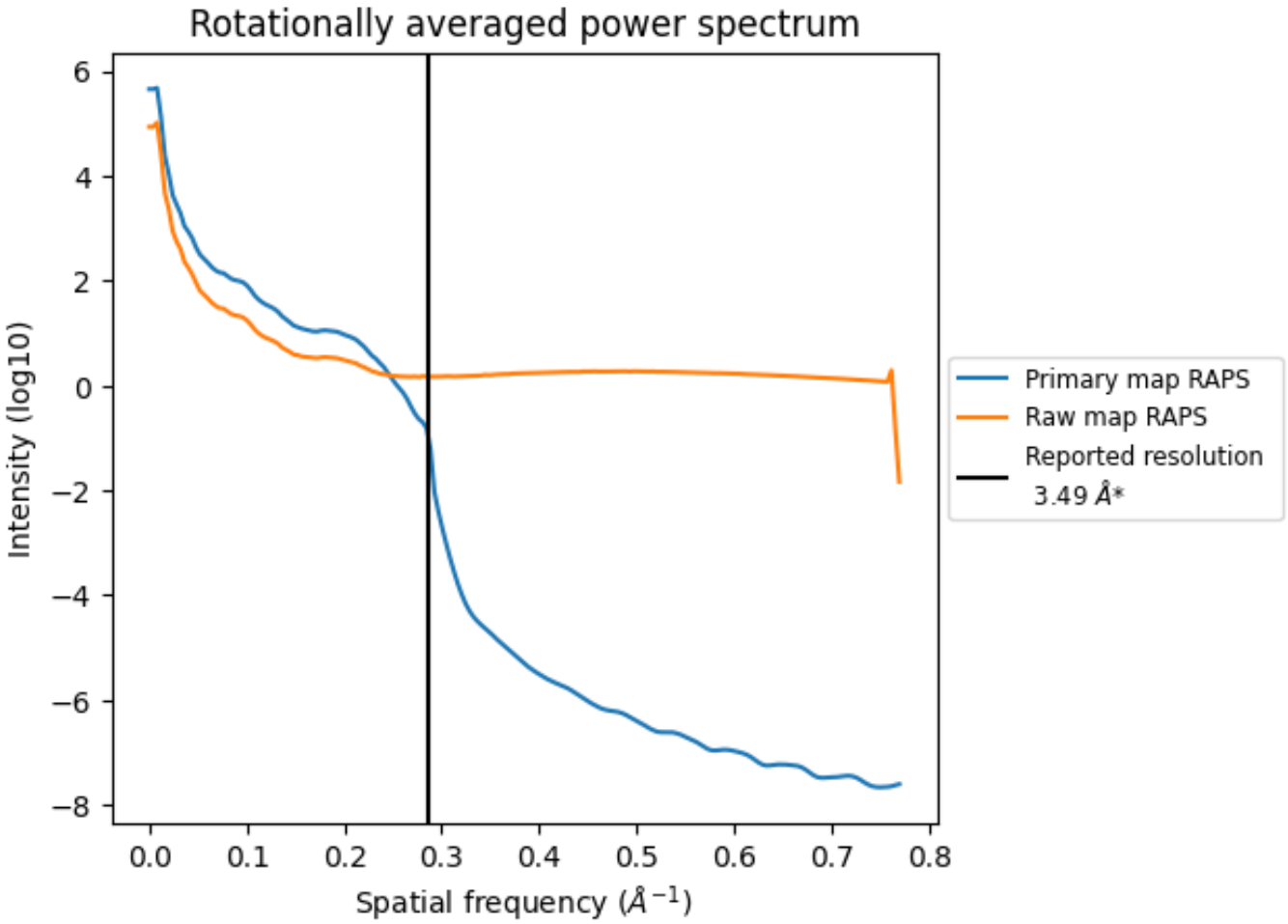
7.2 Volume estimate



The volume at the recommended contour level is 154 nm^3; this corresponds to an approximate mass of 139 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

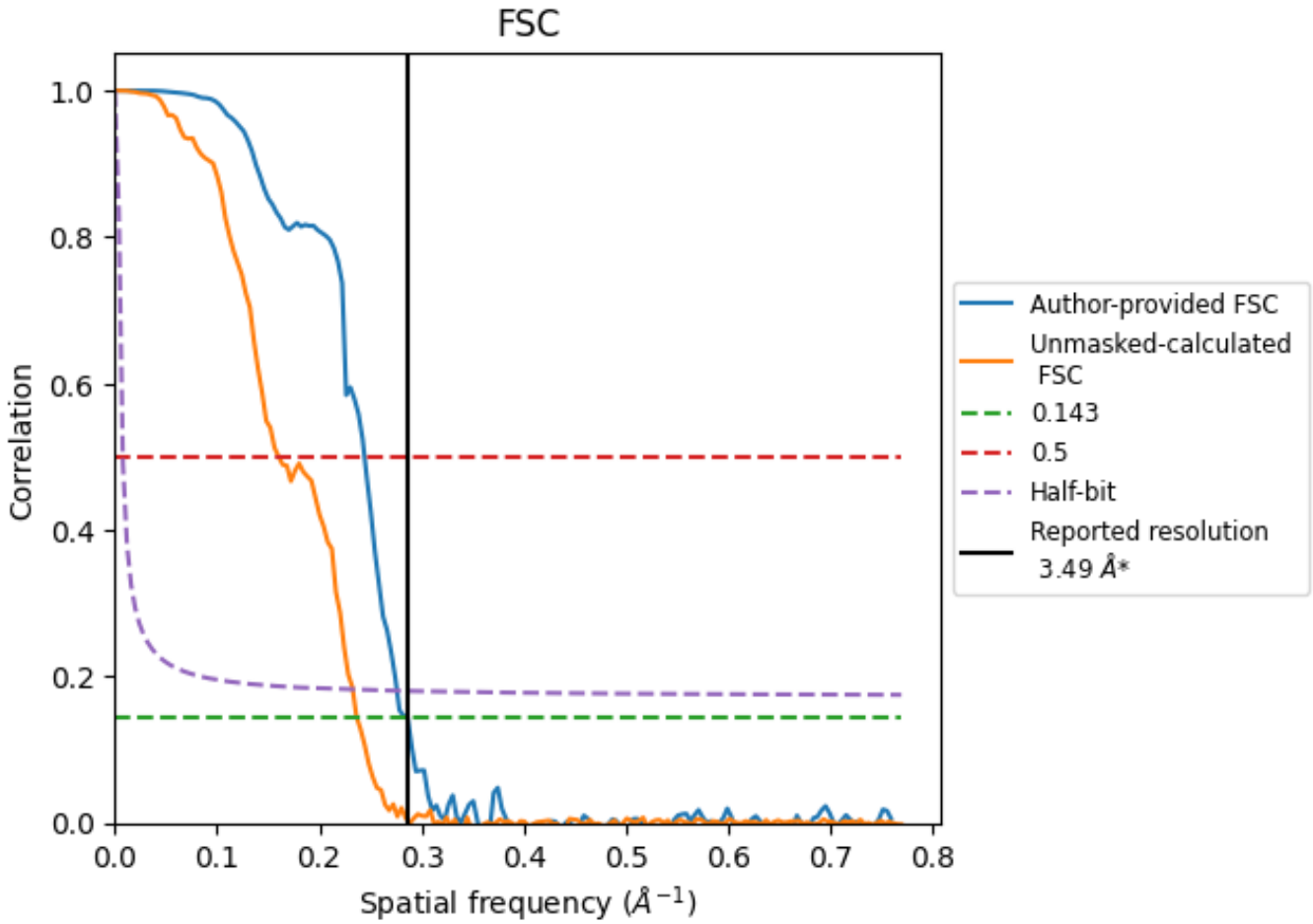


*Reported resolution corresponds to spatial frequency of 0.287 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.287 Å^{-1}

8.2 Resolution estimates (i)

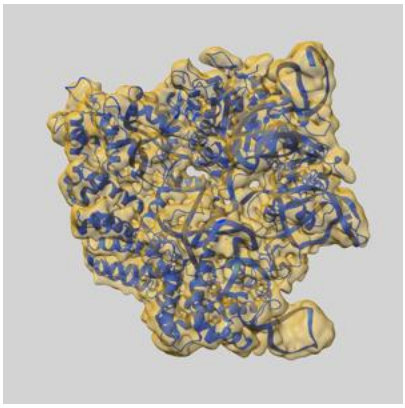
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.49	-	-
Author-provided FSC curve	3.49	4.09	3.62
Unmasked-calculated*	4.22	6.24	4.30

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.22 differs from the reported value 3.49 by more than 10 %

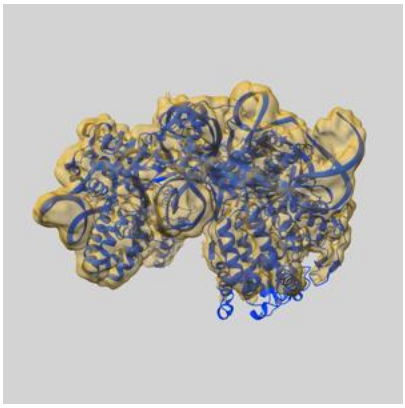
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-14497 and PDB model 7Z4H. Per-residue inclusion information can be found in section 3 on page 4.

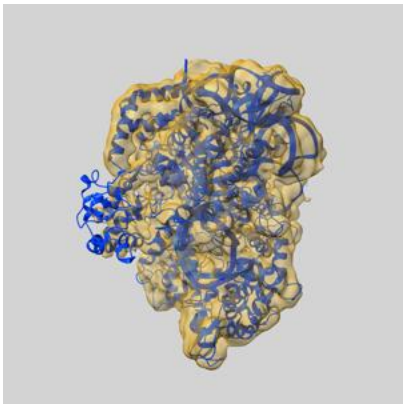
9.1 Map-model overlay



X



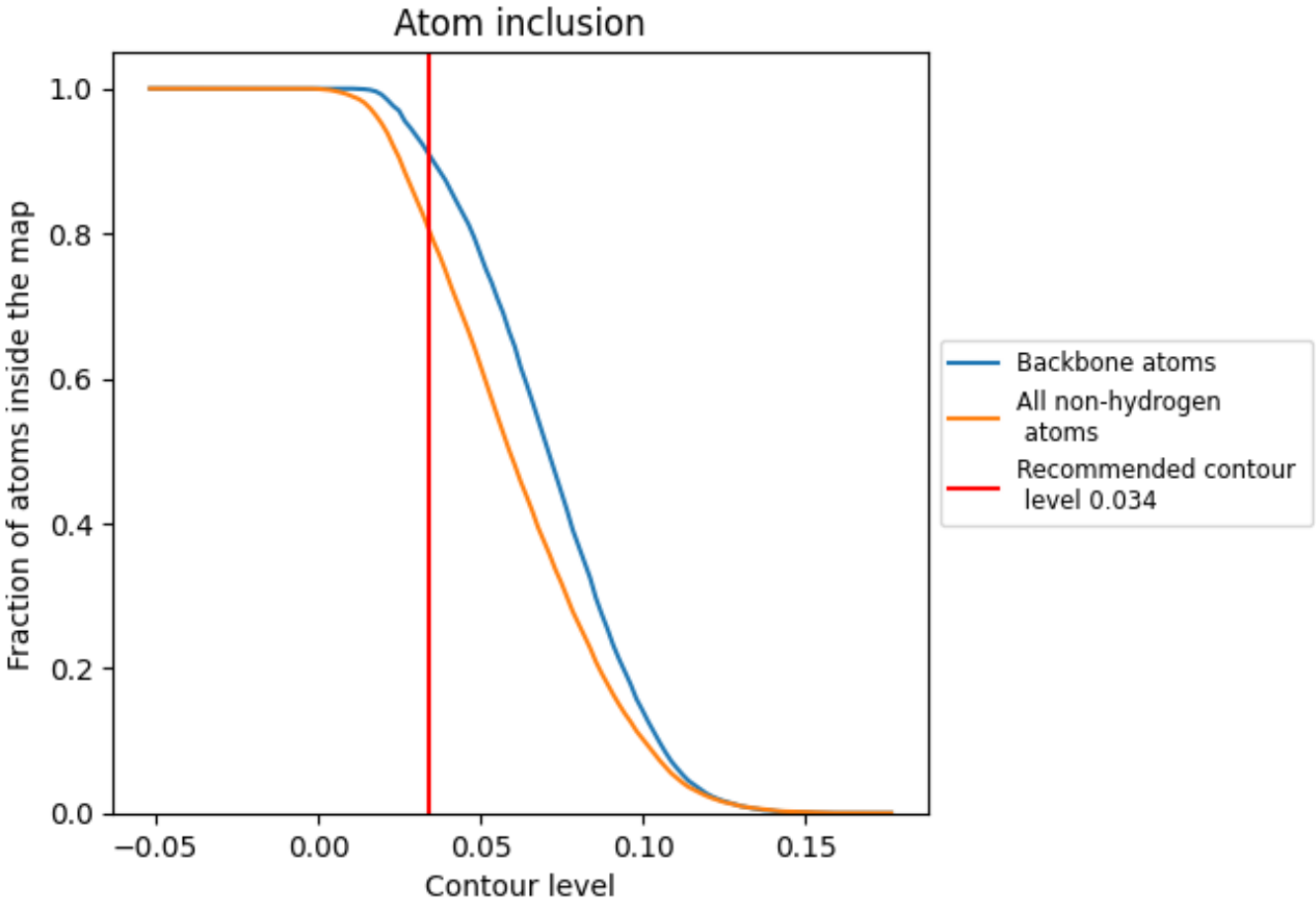
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.034 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Atom inclusion (i)



At the recommended contour level, 91% of all backbone atoms, 81% of all non-hydrogen atoms, are inside the map.